

Preliminary calculation of α_s from Green functions with dynamical quarks

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ABSTRACT: We present preliminary results on the computation of the QCD running coupling constant in the \overline{MS} scheme and Landau gauge with two flavours of dynamical Wilson quarks. Gluon momenta range up to about 7 GeV ($\beta = 5.6, 5.8$ and 6.0) with a constant dynamical-quark mass. This range already allows to exhibit some evidence for a sizable $1/\mu^2$ correction to the asymptotic behaviour, as in the quenched approximation, although a fit without power corrections is still possible with a reasonable χ^2 . Following the conclusions of our quenched study, we take into account $1/\mu^2$ correction to the asymptotic behaviour. We find $\Lambda_{\overline{MS}}^{N_f=2} = 264(27)\text{MeV} \times [a^{-1}(5.6, 0.1560)/2.19\text{GeV}]$, which leads to $\alpha_s(M_Z) = 0.113(3)(4)$. The latter result has to be taken as a preliminary indication rather than a real prediction in view of the systematic errors still to be controlled. Still, being two sigmas below the experimental result makes it very encouraging.

KEYWORDS: Nonperturbative Effects, Quark Masses and SM Parameters, QCD, Lattice QCD.

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The non-perturbative calculation of the running coupling constant of QCD is certainly a very important problem. In pure Yang-Mills it has been performed with several different methods, the most systematic ones using the Schrödinger functional [1], and the gluon Green functions [2]–[5]. It is noticeable that the latter two methods, although very different, end up with perfectly compatible values for Λ_{QCD} .

Of course the real challenge is to compute α_s with dynamical fermions. This task has been undertaken using NRQCD several years ago [7, 8, 9] and, once extrapolated to M_Z leads to rather satisfactory values for $\alpha_s(M_Z)$. Recently, the QCDSF-UKQCD collaboration [10] and the ALPHA one [11] have reported progress in determining α_s with two flavours using relativistic lattice QCD and nonperturbatively improved Wilson fermions.

In this letter we will report our work consisting in applying the Green function method estimate [2]–[5] with non-improved Wilson dynamical quarks. The principle of the method is quite simple since it consists in following the steps which are standard in perturbative QCD in the momentum subtraction scheme. This gives immediately a nonperturbative estimate of the coupling constant at different scales. Its running can be confronted to the perturbative QCD expectation. We use the \widetilde{MOM} renormalization scheme which corresponds to using an asymmetric subtraction point : $p_1^2 = p_3^2 \equiv \mu^2, p_2 = 0$. This scheme proved to give rather good signals and, in spite of the zero momentum, no pathology has been seen.

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From our study of the pure Yang-Mills case [3, 4, 5] we have learnt two main lessons: one is that a study of the asymptotic behaviour of α_s needs a large energy window, since the value of Λ_{QCD} we are looking for depends on the weak logarithmic dependence of α_s on the energy scale μ , the second is that the $1/\mu^2$ correction can be sizable up to a large energy.

We aim at computing α_s , Λ_{QCD} and the power correction term with two flavours of dynamical quarks. This requires, as we shall see in more details, an exploration of the two-dimensional (g_0, m_{sea}) bare parameter space. To this goal we have run lattice simulations on several 16^4 lattices. Notwithstanding the modest volumes of these lattices, we realised that some interesting physics can already be extracted. Furthermore, the exploration of the bare parameter space provides us with new data which might be of interest for unquenched studies by the lattice community. This legitimates in our opinion a progress report which is the aim of this paper.

1. Our strategy

We have computed in the Landau gauge the two-gluon and three-gluon Green functions leading to a nonperturbative calculation of $\alpha_s^{\text{Latt}}(\mu)$ in the well defined MOM schemes [2, 3]. At energies μ above 2.6 GeV we will fit this function by

$$\alpha_s^{\text{Latt}}(\mu^2) = \alpha_{s,\text{pert}}(\mu^2) \left(1 + \frac{c}{\mu^2} \right), \quad (1.1)$$

where $\alpha_{s,\text{pert}}(\mu^2)$ is the perturbative running coupling constant computed to four loops from some fitted Λ_{QCD} , and $\alpha_{s,\text{pert}} c/\mu^2$ is a power correction which has proven, in the $N_f = 0$ case, not to be negligible up to 10 GeV, and was eventually traced back to an OPE condensate $\langle A_\mu A^\mu \rangle$. The reason for choosing as in eq. (1.1) a non perturbative correction $\propto \alpha_{s,\text{pert}}(\mu^2)/\mu^2$ instead of simply $\propto 1/\mu^2$ is twofolds:

- (i) Theoretically, an OPE study [5] including a computation of the anomalous dimension of the coefficient of $\langle A^2 \rangle$ leads to an expected energy dependence close to $\alpha_{s,\text{pert}}(\mu^2)/\mu^2$;
- (ii) Practically in the quenched as well as unquenched case the fit with $\alpha_{s,\text{pert}}(\mu^2)/\mu^2$ is much more stable for changes of the energy window than the fit with $1/\mu^2$. The former stability will be illustrated in table 2.

Interestingly, α_s^{Latt} is at the same time both the goal of our study and a very useful tool: from the lattice simulations one extracts the continuum α_s up to small lattice artifacts; lattice spacing ratios are then fitted to preserve the continuity of $\alpha_s(\mu)$ for the whole set of data.

This program is performed on hypercubic lattices in order to simplify the necessary tensorial analysis of the Green functions.¹ In the $N_f = 0$ case we combined $\beta = 6.0, 6.2, 6.4, 6.8$

¹This does not allow to compute the ρ meson mass, which is better performed on lattices longer in time direction than in space. Some consequences will be discussed later.

quenched lattice simulations, i.e. a lattice spacing ranging from ~ 0.03 fm to 0.1 fm, in [3, 5], allowing to reach momenta up to 10 GeV.

With dynamical fermions the physics depends on two parameters, β which represents the bare coupling constant and κ_{sea} representing the bare dynamical-quark mass. A wide energy window is reached by combining simulations with different lattice spacings and the same *renormalised dynamical-quark mass expressed in physical units*. The problem is of course that we do not know a priori for a given β which κ_{sea} corresponds to one given renormalised dynamical-quark mass in physical units. This needs as mentioned above some exploration of the $(\beta, \kappa_{\text{sea}})$ parameter space to find one or several lines of equal dynamical masses. In view of the computational cost of such an exploration we have chosen to perform it on a small volume, 16^4 .

We now would like to sketch our strategy to compute the lattice spacings and the renormalised dynamical-quark masses in this exploratory stage on a 16^4 volume. We proceed as follows. We start from a calibrating set of parameters $(\beta, \kappa_{\text{sea}})$ for which some published results yield the inverse lattice spacing a^{-1} computed from some hadronic quantity, for example the ρ meson mass. We then estimate a^{-1} for other values of $(\beta, \kappa_{\text{sea}})$ by matching² the value of $\alpha_s(\mu)$. This uses as an assumption that we may neglect the dependence of α_s on the dynamical-quark mass, at least in the mass range under consideration. This assumption is not more arbitrary than any other calibration based on, for example, the physical ρ meson mass, which neglects the unknown dependence of the ρ meson mass on the dynamical-quark mass.

Once we have estimated the lattice spacings for all our lattices with different sets $(\beta, \kappa_{\text{sea}})$, we estimate m_{sea} from the ratio $\partial_\mu A^\mu / P_5$ where A^μ is the axial current and P_5 the pseudoscalar density, computed for a valence quark³ with the same bare mass as the dynamical quark ($\kappa_{\text{val}} = \kappa_{\text{sea}}$).

At the end of this procedure we can fix with a reasonable accuracy a set of couples $(\beta, \kappa_{\text{sea}})$ which includes our calibrating lattice and for which the dynamical-quark mass remains constant in physical units when β is varied. This knowledge allows for a preliminary analysis of α_s with two flavours, of the resulting $\Lambda_{\overline{\text{MS}}}^{N_f=2}$ and power correction term, and finally of $\alpha_s(M_Z)$. This will be presented in this letter.

Still we do not forget that finite volume effects may be large in such a small volume, that our dynamical-quark masses are large, etc. We will therefore briefly discuss sources of systematic uncertainties at the end of this letter. We are however now in a position to launch the calculations on a larger volume 24^4 and/or with lighter masses and correct for the biases of our present results.

2. Some useful perturbative formulae

We now proceed to establish the conventions and to introduce the formulae that we will

²Our matching procedure was proved to be succesful when applied to quenched data, where lattice spacings are well known [6].

³We call valence quarks the quarks which contribute to the current densities and propagate in the gauge field background. The latter depends on the sea quark mass. The theory is unitary only if valence and sea quarks have the same mass. However we will also make use of $\kappa_{\text{val}} \neq \kappa_{\text{sea}}$ as an intermediate step.

use in the following. $\alpha_{\text{s,pert}}(\mu^2)$ in eq. (1.1) stands for the perturbative running coupling constant expanded up to the fourth loop and verifying (in this section we write α instead of $\alpha_{\text{s,pert}}(\mu^2)$ to simplify the notations)

$$\frac{d}{d \ln \mu} \alpha = - \left(\frac{\beta_0}{2\pi} \alpha^2 + \frac{\beta_1}{4\pi^2} \alpha^3 + \frac{\beta_2}{64\pi^3} \alpha^4 + \frac{\beta_3}{128\pi^4} \alpha^5 \right). \quad (2.1)$$

In all schemes

$$\beta_0 = 11 - \frac{2}{3} N_f \quad \beta_1 = 51 - \frac{19}{3} N_f, \quad (2.2)$$

while β_2, β_3 depend on the particular scheme. The values we need for the $\widetilde{\text{MOM}}$ scheme can be found in ref. [12]. The exact integration of eq. (2.1) to the third loop, with the standard boundary condition defining the Λ parameter [13], leads to [3]

$$\begin{aligned} \Lambda^{3\text{loops}} &= \Lambda^{(c)}(\alpha) \left(1 + \frac{\beta_1 \alpha}{2\pi \beta_0} + \frac{\beta_2 \alpha^2}{32\pi^2 \beta_0} \right)^{\frac{\beta_1}{2\beta_0^2}} \times \\ &\times \exp \left\{ \frac{\beta_0 \beta_2 - 4\beta_1^2}{2\beta_0^2 \sqrt{\Delta}} \left[\arctan \left(\frac{\sqrt{\Delta}}{2\beta_1 + \beta_2 \alpha / 4\pi} \right) - \arctan \left(\frac{\sqrt{\Delta}}{2\beta_1} \right) \right] \right\}, \quad (2.3) \end{aligned}$$

where $\Lambda^{(c)}$ denotes the conventional two loops formula:

$$\Lambda^{(c)} \equiv \mu \exp \left(\frac{-2\pi}{\beta_0 \alpha} \right) \times \left(\frac{\beta_0 \alpha}{4\pi} \right)^{-\frac{\beta_1}{\beta_0^2}}; \quad (2.4)$$

and $\Delta \equiv 2\beta_0 \beta_2 - 4\beta_1^2 > 0$ in the $\widetilde{\text{MOM}}$ scheme which we use. If one only retains the first correction coming from the perturbative fourth loop, it can then be written

$$\Lambda^{4\text{loops}} = \Lambda^{3\text{loops}} \exp \left(-\frac{\beta_3}{64\pi^2 \beta_0^2} \alpha^2 \right). \quad (2.5)$$

In the previous formula, of course, the use of Λ , α and β 's stands for the Λ parameter, the running coupling constant and beta function coefficients in the particular $\widetilde{\text{MOM}}$ renormalisation scheme. From now on we will systematically convert Λ into $\Lambda_{\overline{\text{MS}}}$ using [3]

$$\Lambda_{\overline{\text{MS}}} = \Lambda \exp \left[-\frac{1}{22} \left(\frac{70}{3} - \frac{22}{9} N_f \right) \right]. \quad (2.6)$$

No analytical expression can exactly inverse neither three-loop eq. (2.3) nor four-loop eq. (2.5). The following formula gives nevertheless an approximated solution to the inversion of the perturbative expansion of eq. (2.5):

$$\begin{aligned} \alpha_{\text{s,pert}}(\mu^2) &= \frac{4\pi}{\beta_0 t} - \frac{8\pi \beta_1}{\beta_0} \frac{\log(t)}{(\beta_0 t)^2} + \\ &+ \frac{1}{(\beta_0 t)^3} \left(\frac{2\pi \beta_2}{\beta_0} + \frac{16\pi \beta_1^2}{\beta_0^2} (\log^2(t) - \log(t) - 1) \right) + \frac{1}{(\beta_0 t)^4} \times \\ &\times \left[\frac{2\pi \beta_3}{\beta_0} + \frac{16\pi \beta_1^3}{\beta_0^3} \left(-2 \log^3(t) + 5 \log^2(t) + \left(4 - \frac{3\beta_2 \beta_0}{4\beta_1^2} \right) \log(t) - 1 \right) \right], \quad (2.7) \end{aligned}$$

where $t = \log(\mu^2/\Lambda^2)$. The exact numerical inversions of, for instance, eq. (2.5), can be easily obtained; but, of course, such an exact inversion and the approximated solution in eq. (2.7) should only differ by perturbative contributions of order higher than four loops.

β	κ_{sea}	Volume	κ_{pc}	a^{-1} (GeV)	m_{sea} (MeV)
5.6 [14]	0.1560	$16^3 \times 32$		2.19(8)	
5.6 [14]	0.1575	$16^3 \times 32$		2.38(7)	
5.6 [15]	0.1575	$24^3 \times 40$	0.15927(5)	2.51(6)	
5.6 [15]	0.1580	$24^3 \times 40$	0.15887(4)	2.54(6)	
5.6	0.1560	24^4	0.16053(3)	2.19(8)	164(7)
5.6	0.1560	16^4	0.16048(13)	2.19(8)	164(7)
5.6	0.1575	16^4	0.1593(1)	2.42(9)	79(3)
5.8	0.1500	16^4	0.15672(6)	2.45(13)	325(18)
5.8	0.1525	16^4	0.15555(12)	2.76(7)	173(4)
5.8	0.1535	16^4	0.15522(9)	2.91(18)	103(16)
5.8	0.1540	16^4	0.15499(6)	3.13(13)	64(5)
6.0	0.1480	16^4	0.15272(7)	3.62(10)	391(12)
6.0	0.1490	16^4	0.15262(7)	3.73(13)	308(12)
6.0	0.1500	16^4	0.15238(4)	3.78(14)	213(3)
6.0	0.1505	16^4	0.15240(5)	3.84(15)	169(8)
6.0	0.1510	16^4	0.15207(3)	3.96(16)	96(4)

Table 1: Data taken from literature and first iteration estimates from our runs. κ_{pc} is defined in subsection 3.3. The dynamical-quark masses are renormalised in the $\overline{\text{MS}}$ scheme at 3 GeV.

3. The First iteration

3.1 Lattice spacings

The lattice parameters which we have used for our simulations are displayed in table 1 together with our estimates of the pseudocritical κ 's, κ_{pc} , defined in subsection 3.3, of the the lattice spacings and of the sea quark masses.

We will not repeat the method used to extract α_s from $\widehat{\text{Green}}$ functions as it is exactly similar to what was done in the pure Yang-Mills case. The $\widehat{\text{MOM}}$ scheme uses the “asymmetric” three point Green function, i.e. with gluon squared momenta $(0, \mu^2, \mu^2)$ where $\mu^2 = n(2\pi/L)^2$, n being an integer.⁴ Let us nevertheless recall that the “asymmetric” three-point Green function turned out to be more convenient for our purpose than the symmetric one (i.e. with gluon square momenta (μ^2, μ^2, μ^2)): the high accuracy achieved in our quenched study [2, 3, 4, 5] gave us some evidence that the “asymmetric signal” was less noisy than the symmetric one, while being as reliable (more momenta available and no observable infrared pathology due to the zero momentum).

In table 1, we give the full set of runs performed and the preliminary values obtained for a^{-1} and m_{sea} . In the first four rows, we also quote sets of values taken from literature [14, 15]. In particular, the value $a^{-1} = 2.19(8)$ GeV for (5.6, 0.1560) is taken from [14] and we will use it to calibrate all our runs. As already mentioned, ratios of lattice spacings result from imposing the continuity of $\alpha_s(\mu)$ from different lattices, neglecting the expected

⁴Any integer verifies $n = \sum_{i=0,3} n_i^2$ for at least one set of integers $n_i, i = 0, 3$ (Lagrange’s four-square theorem).

small dependence of α_s on the dynamical mass m_{sea} . Since the error on the calibrating a^{-1} propagates trivially to Λ_{QCD} we will use 2.19 GeV without its error until eq. (4.2); a discussion of these errors will follow eq. (4.2). Thus the errors quoted here for a^{-1} only stand for the ratios.

3.2 Sea-quark masses

Once the lattice spacings are estimated, we also need to compute am_{sea} . To this aim we compute the propagators of valence quarks for several κ_{val} among which one with $\kappa_{\text{val}} = \kappa_{\text{sea}}$ in order to be able to deduce the mass of the sea quark from the estimated mass of the valence quark.

This is done using the ratio

$$\rho = \frac{1}{2} \frac{\sum_{\vec{x}} P_5(0) \partial_0 A_0(\vec{x}, t)}{\sum_{\vec{x}} P_5(0) P_5(\vec{x}, t)}, \quad (3.1)$$

where P_5 is the pseudoscalar density, and A_μ the axial current.

To estimate the ratio ρ in (3.1) we have used two methods. The simplest consists in looking for a plateau of the ratio, the time derivative in the numerator being computed by a symmetrised discrete difference. However this “brute-force” estimate appeared to be affected by some strong $O(a)$ effects in several cases.

The second method, which is a variant of the one proposed in [16], fits on some time interval the $\langle P_5 P_5 \rangle$ in the denominator by a cosh function and the $\langle P_5 A_0 \rangle$ in the numerator by a sinh with the same “mass” term.⁵ The time derivative of the sinh in the numerator is then proportional to the cosh in the denominator and the ratio gives an estimate of the ratio ρ in (3.1). We have used the second method because it turned out to be more stable against the change of parameters (domain of the fit) and to provide a better continuity when κ is changed.

The valence mass is given by

$$am_{\text{val}} = \frac{Z_A}{Z_P} \rho. \quad (3.2)$$

For Z_A and Z_P in the RI-MOM scheme, we have taken [17] $Z_A = 0.77(1)$ and $Z_P = 0.54(1)$ i.e. $Z_A/(2Z_P) \simeq 0.71$ at $\mu = 3 \text{ GeV}$ (the value of Z_P is derived from the Ward identity value of Z_P/Z_S [18]). The large Goldstone pole contribution stressed in ref. [19] is claimed⁶ to be eliminated in this value of Z_P . A more careful study of the renormalization constant will be performed soon.

From am_{sea} and a^{-1} we extract the masses presented in table 1. These masses are computed in the $\overline{\text{MS}}$ scheme (3 GeV); the conversion from RI-MOM to $\overline{\text{MS}}$ is obtained by using formulae involving the four-loop anomalous dimensions of the quark mass [20].

⁵It is not really a mass since the very short time interval considered does not allow to isolate the ground state. It nevertheless turns out that the data for $5 \leq t \leq 11$ can be satisfactorily fitted respectively with a cosh and a sinh.

⁶Indeed, in ref. [23] this method is applied and agrees with ref. [24], obviously free of Goldstone boson contribution. Although the Goldstone boson question is not commented in [23] this seems to confirm the above-mentioned claim.

3.3 Pseudocritical κ : κ_{pc}

For any parameter set (β, κ_{sea}) , having computed the valence masses for several values of κ_{val} we extrapolate to a vanishing valence mass. We call “pseudocritical κ ”, $\kappa_{pc}(\kappa_{sea})$, the value of κ_{val} for which $m_{val} = 0$. The values of am_{val} as a function of $1/\kappa_{val}$ are perfectly compatible with linear fits.

The pseudocritical κ 's as a function of $1/\kappa_{sea}$ are also compatible with a linear fit except for one point at $\beta = 6.0$: $\kappa_{sea} = 0.1510$. We did not succeed to understand the reason for this unusual behaviour and have for the moment withdrawn this point from our fit for $\beta = 6.0$. We call “critical κ ” ($\kappa_c(\beta)$) for one β the value of κ_{sea} at which the extrapolated κ_{pc} is equal to κ_{sea} : $\kappa_{pc}(\kappa_c) = \kappa_c$.

Our results for κ_c are the following:

$$\kappa_c(5.6) = 0.158480(32), \quad \kappa_c(5.8) = 0.154682(34), \quad \kappa_c(6.0) = 0.152012(34). \quad (3.3)$$

At $\beta = 5.6$, we made the extrapolation using two runs performed by us, ($\kappa_{sea} = 0.1575$ and $\kappa_{sea} = 0.1560$ (24^4)) and a third one at $\kappa_{sea} = 0.1580$ taken from [15]. The value of $\kappa_c(5.6)$ we obtained is perfectly compatible with the one ($\kappa_c(5.6) = 0.15846(5)$) published by SESAM [14]. Replacing our run on 24^4 by the one on 16^4 induces no significant difference. To our knowledge, the last two values are new.

3.4 Some tests of finite volume effects

It is clear that a critical point in everything we report here is the risk that finite volume effect might spoil our results. In our mind the present work should be mainly a preparation for similar runs on larger volumes (24^4) and we want to be sure that the information gathered on 16^4 is relevant enough to tune our parameters for a larger volume. We performed two checks with this purpose.

The first one is the comparison of the two runs at $\beta = 5.6, \kappa_{sea} = 0.1560$ reported in table 1. It can be seen that there is no significant difference between the results for 16^4 and 24^4 .

The second one relies on the idea that there could be some kind of first order phase transition at very small volume, a deconfinement and/or chiral restoration transition. Chiral symmetry restoration has the effect of eliminating the Goldstone boson and thus of invalidating the relation $m_P^2 \propto (m_q + m_{\bar{q}})$ where m_P is the lightest pseudoscalar meson “mass”⁷ and m_q ($m_{\bar{q}}$) the (anti)quark mass.

Our analysis has found empirically that all our lattice data⁷ can be fitted to a good accuracy by the following formula:

$$m_P^2 = 2Bm_{sea} + \frac{r}{V}. \quad (3.4)$$

Here $m_q = m_{\bar{q}}$ is the dynamical-quark mass, and V the lattice volume, both expressed in

⁷We included the run at $\beta = 6.0, \kappa_{sea} = 0.1510$ in this analysis to test in a different way its chiral behaviour; however it did not exhibit any pathology here.

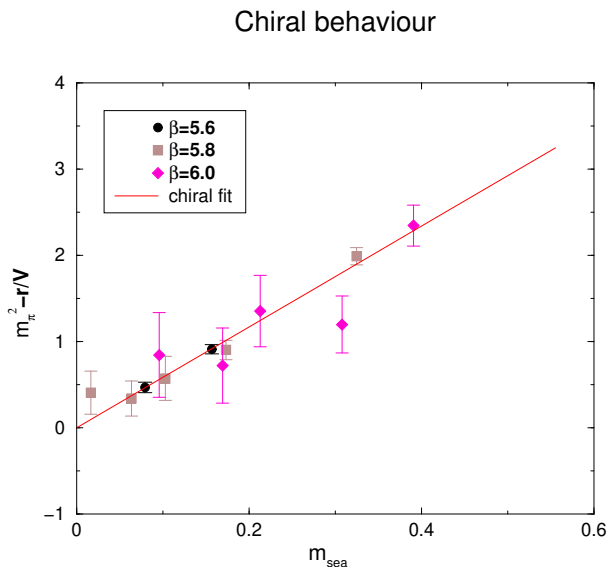


Figure 1: Finite size effects on chiral behaviour.

physical units. We still take the quark mass renormalised in the $\overline{\text{MS}}$ scheme at 3 GeV. We then obtained

$$B = 2.74(5) \text{ GeV}, \quad r = 1.41(5) \text{ GeV}^2 \text{ fm}^4; \tag{3.5}$$

from a best fit with a $\chi^2/\text{d.o.f.} = 0.57$ (see figure 1).

Eq. (3.5) shows a strong but smooth finite volume effect⁸, without any sign of a sudden change of regime, as would be the case with a first order phase transition.

In the infinite volume limit we should recover the pseudoscalar mass $m_{P,\infty}$. Indeed we checked for $\beta = 5.6$ and $\kappa_{\text{sea}} = 0.1575$ that $m_{P,\infty}^2 \simeq 0.432(18) \text{ GeV}^2$, in good agreement with SESAM [14]: $m_P^2 \simeq 0.432(9) \text{ GeV}^2$. Furthermore $m_{P,\infty}^2 = 2.74(m_q + m_{\bar{q}})$, which from the pion mass gives $(m_u + m_d)/2 \simeq 3.6 \text{ MeV}$ and from the kaon mass $m_s \simeq 90 \text{ MeV}$ at 3 GeV. This compares fairly well to other lattice estimates.

4. Second iteration: fitting Λ_{QCD} and power corrections

4.1 Fitting Λ_{QCD} and $O(1/\mu^2)$ coefficient

Once we have an approximate estimate of the lattice spacings and dynamical masses, we now proceed with a combined fit of α_s on the line with approximately constant dynamical-quark mass which goes through $\beta = 5.6, \kappa_{\text{sea}} = 0.1560$: $\beta = 5.8, \kappa_{\text{sea}} = 0.1525$ and $\beta = 6.0, \kappa_{\text{sea}} = 0.1505$. This allows to reach momenta as large as $\sim 7.0 \text{ GeV}$, large enough to see the asymptotic behaviour, provided we take into account $O(1/\mu^2)$ corrections.

According to our ansatz (1.1), we need to fit simultaneously the lattice spacing ratios, and the parameters Λ_{QCD} and c (coefficient of $\alpha_{s,\text{pert}}/\mu^2$). To fit the lattice spacings one

⁸We cannot compare our finite volume correction in eq. (3.4) to existing theoretical studies of finite volume effects on ground state energies [21]: indeed, as already stressed, m_P is not really a ground state energy.

μ_{\min} (GeV)	$\Lambda_{\overline{\text{MS}}}$ (MeV)	c (GeV ²)	$\chi^2/\text{d.o.f.}$
2.6	264(24)	2.66(77)	0.58
3.1	256(20)	3.03(85)	0.56
3.6	267(29)	2.51(1.21)	0.54
4.1	269(29)	2.44(1.75)	0.71

Table 2: Four-loop fit with power corrections, eq. (1.1), on varying energy windows ($> \mu_{\min}$). The stability of the fit is fairly good.

needs some analytic function to interpolate between the measured points and to adjust its parameters simultaneously with the lattice spacings to the smallest χ^2 . Two approaches are possible.

One approach is to use the asymptotic four loops behaviour plus $\alpha_{\text{s,pert}}/\mu^2$ corrections as the analytic function. This would allow to reach both goals with one stroke but at the expense of eliminating about one half of the points at $\beta = 5.6, \kappa_{\text{sea}} = 0.1560$ which are too low in energy to follow the asymptotic behaviour.

The other approach proceeds in two steps as follows. To fit the lattice spacings we have used polynomials. At $\beta = 5.6, \kappa_{\text{sea}} = 0.1560$ we have used both the 16^4 and the 24^4 lattices. A universal polynomial (figure 2, *Matching of lattice spacings*) fitting all points of the four lattice settings considered does indeed exist except for a few points which happen to correspond to $n = (L\mu)^2/(4\pi^2) \lesssim 2 - 4$ where L is the length of the lattice. We attribute this behaviour to a strong finite volume effect [3] and exclude the points below some IR cutoff. Varying this IR cut from $n > 2$ to $n > 4$ leads to a variation in χ^2 from $\chi^2/\text{d.o.f.} = 1.06$ to $\chi^2/\text{d.o.f.} = 0.79$. For lower IR cut-offs the χ^2 increases dramatically, while for higher IR cut-offs too many points are excluded. The uncertainty induced by the choice of the cutoff is taken into account in the systematic error which affects the values quoted below. At this point, it should perhaps be emphasized again that this procedure was tested on quenched data, providing us with the generally admitted lattice spacing ratios. In this way we obtain:

$$\begin{aligned}
 a^{-1}(5.8, 0.1525) &= 2.85 \pm .09 \pm .04 \times \frac{a^{-1}(5.6, 0.1560)}{2.19 \text{ GeV}} \text{ GeV} \\
 a^{-1}(6.0, 0.1505) &= 3.92 \pm .11 \pm .07 \times \frac{a^{-1}(5.6, 0.1560)}{2.19 \text{ GeV}} \text{ GeV}, \quad (4.1)
 \end{aligned}$$

where the central value corresponds to a cut at $n \geq 3$, the first error is statistical and the second is systematic. From now on, we are going to use these ratios, correcting the first iteration estimates shown in table 1.

Once the lattice spacings have been estimated we perform a combined fit of $\Lambda_{\overline{\text{MS}}}^{N_f=2}$ and the coefficient c as defined in eq. (1.1) with $\alpha_{\text{s,pert}}^{N_f=2}$ given by the r.h.s. of eq. (2.7). The result is plotted in figure 2, (*Asymptotic fit of α_s*).

From the results in table 2 we conclude:

$$\Lambda_{\overline{\text{MS}}}^{N_f=2} = 264(27) \frac{a^{-1}(5.6, 0.1560)}{2.19 \text{ GeV}} \text{ MeV} \quad c = 2.7(1.2) \left[\frac{a^{-1}(5.6, 0.1560)}{2.19 \text{ GeV}} \text{ GeV} \right]^2, \quad (4.2)$$

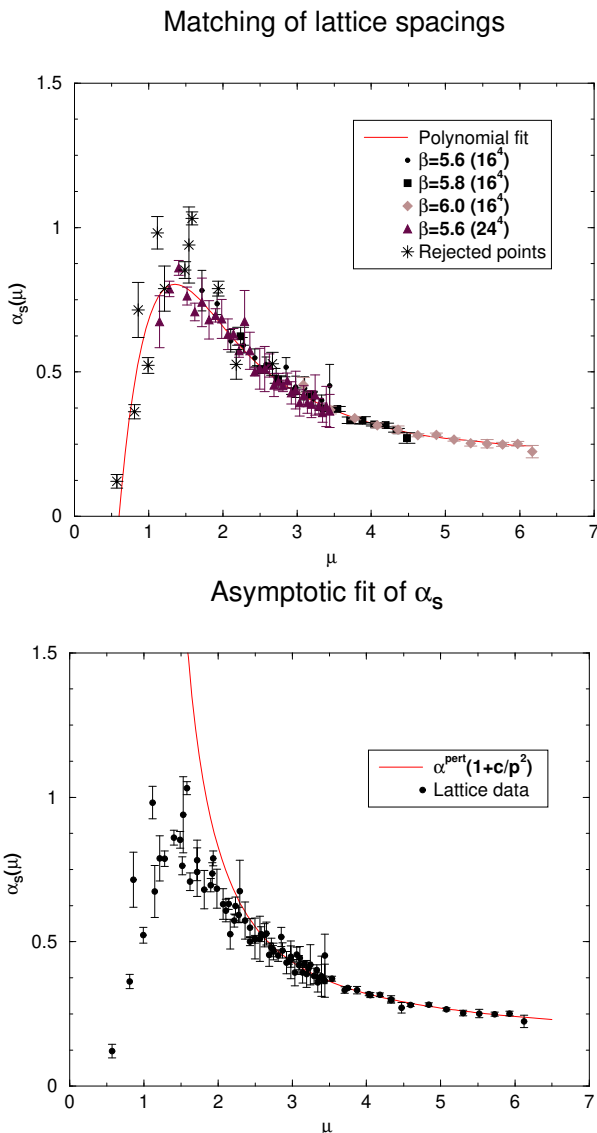


Figure 2: Fits of α_s obtained with four lattices.

The same analysis using the formula in eq. (1.1) leads to

$$\Lambda_{\overline{\text{MS}}}^{N_f=0} \simeq 252(10)\text{MeV} \quad c = 1.0(1)\text{GeV}^2 \quad (4.3)$$

from our $N_f = 0$ data⁹ [3].

If we use the first approach mentioned above, i.e. fitting from the beginning with the formula of eq. (1.1), the result are perfectly compatible with eqs. (4.1) and (4.2). If we try the same procedure without power corrections, keeping an energy window ranging from

⁹If the fit for $N_f = 0$ is performed according to $\alpha_s^{\text{Latt}}(\mu^2) = \alpha_{s,\text{pert}}(\mu^2) + \frac{c}{\mu^2}$ instead of eq. (1.1) the result is $\Lambda_{\overline{\text{MS}}}^{N_f=0} \simeq 237(10)\text{MeV}$ [4].

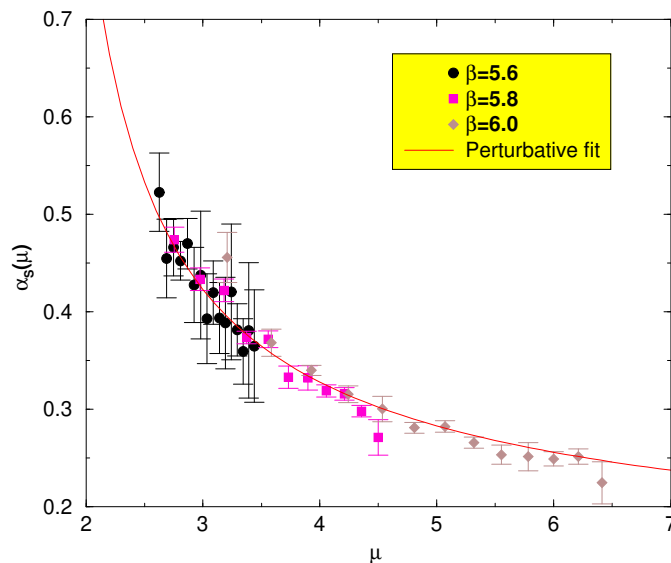


Figure 3: Purely perturbative fit of α_s .

2.6 GeV, we can obtain a best fit with the following parameters (see figure 3):

$$\begin{aligned}
 a^{-1}(5.8, 0.1525) &= 2.86(6) \times \frac{a^{-1}(5.6, 0.1560)}{2.19 \text{ GeV}} \text{ GeV} \\
 a^{-1}(6.0, 0.1505) &= 4.08(9) \times \frac{a^{-1}(5.6, 0.1560)}{2.19 \text{ GeV}} \text{ GeV}
 \end{aligned}
 \tag{4.4}$$

and

$$\Lambda_{\overline{\text{MS}}}^{N_f=2} = 345(6) \quad \chi^2/d.o.f. = 0.96.
 \tag{4.5}$$

It is not surprising that $\Lambda_{\overline{\text{MS}}}^{N_f=2}$ is larger when the fit does not include $1/\mu^2$ corrections, since the parameters $\Lambda_{\overline{\text{MS}}}^{N_f=2}$ and c vary naturally a contrario: if one increases the other decreases. There is a possible contradiction between the acceptable χ^2 found in (4.5) and the fact that in eq. (4.2) the coefficient c is three standard deviations away from 0. This might be due to some correlations in the data; further study is needed to settle the origin of the discrepancy.

Let us nevertheless underline three facts that make us confident about the pertinence of incorporating power corrections:

1. The OPE analysis [5] still holds in the unquenched case, so we theoretically expect the presence of power corrections; we wonder about their magnitude.
2. In the pure Yang-Mills case [3, 4, 5] where high accuracy computations were achieved, the purely perturbative formula could not provide us with a good fit, but the one including power corrections managed to. This “numerical evidence” is comforted by the good agreement of our value of $\Lambda_{\overline{\text{MS}}}^{N_f=0}$ and that of the ALPHA collaboration [5, 24].

3. Provided we do control the systematic uncertainties, the current data already show a tendency to discriminate in favour of the inclusion of non-perturbative terms. Indeed, in the case of a fit *without* power corrections, the lattice data are lying *over* the fitting curve for the lowest values of our energy window, and *under* the curve for the highest energy values. We expect this tendency to become clearer with higher statistics.

Of course, we are conscious that the present letter would benefit from a deeper discussion of systematic errors. In particular the use of non-improved dynamical quarks leads to $O(a)$ errors. However our lattice spacings are all rather small and these errors partly cancel in the ratios of lattice spacings. The dominant error is thus an overall $O(a)$ error on the calibrating lattice spacing. This error propagates multiplicatively to the values of $\Lambda_{\overline{\text{MS}}}^{N_f=2}$ and c . We are not in a position at the moment to estimate in a reliable way this systematic error. A rough estimate can be obtained either by analogy with the quenched case, looking at [25, figure 4] for $a^{-1} \sim 2.2 \text{ GeV}$ or directly in the unquenched case from [14, figure 2]. A crude estimate is 20%. This would give 50 MeV on $\Lambda_{\overline{\text{MS}}}^{N_f=2}$. The effect on $\alpha_s(M_Z)$ will be a systematic error of ± 0.004 .

It is useful to notice that the $O(a)$ errors are $O(am_{\text{sea}})$ or $O(a\Lambda_{\text{QCD}})$. No errors $O(a\mu)$ are expected due to symmetry reasons: the hypercubic symmetry of the lattice ($\mu_\nu \rightarrow -\mu_\nu$ for any ν) implies that the momentum dependent errors are $O(a^2\mu^2)$, exactly as in the pure Yang-Mills case. We did not see any significant effect of the latter errors for the momenta that we have considered. In particular such errors should show up in figure 2 as a systematic deviation from the global fit for the data with largest $a^2\mu^2$.

4.2 Estimating $\alpha_s(M_Z)$

At an energy of the order of the Z meson mass the $O(1/\mu^2)$ power correction becomes irrelevant. We will therefore only keep $\alpha_{\text{s,pert}}$, the perturbative part of α_s from our fit and extrapolate. We proceed as indicated in [13]. We start from an energy of 1.3 GeV, the $\overline{\text{MS}}$ charm mass which is taken as the charm threshold.¹⁰ At such an energy we will extrapolate from our quenched and two-flavour results to three flavours. We then start evolving up with four flavours to the beauty threshold, 4.3 GeV, and then further up with 5 flavours to M_Z .

Applying eqs. (2.3)–(2.7) with the values of $\Lambda_{\overline{\text{MS}}}$ in eqs. (4.2) and (4.3) and assuming $a^{-1}(5.6, 0.1560) = 2.19 \text{ GeV}$ we get in $\overline{\text{MS}}$ scheme

$$\alpha_{\text{s,pert}}^{N_f=0}(1.3) = 0.259(6), \quad \alpha_{\text{s,pert}}^{N_f=2}(1.3) = 0.306(20), \quad \alpha_{\text{s,pert}}^{N_f=3}(1.3) = 0.329(26), \quad (4.6)$$

where the $N_f = 0, 2$ results come from direct lattice estimates in [3] and in this work, while the $N_f = 3$ has been extrapolated from the two latter.¹¹

¹⁰We have preferred to follow the tradition here, although it is not clear to us why one should use the $\overline{\text{MS}}$ mass and not the pole mass, and why the threshold is at m_c and not $2m_c$ where the charm loop dispersive contribution starts for the gluon propagator.

¹¹We simply assume that the extrapolation to an odd number of flavors is legitimate, not knowing what to do better.

The evolution up to M_Z (where non-perturbative corrections are negligible) and down to M_τ gives

$$\alpha_s(M_Z) = 0.113(3)(4) \quad \alpha_{s,\text{pert}}(M_\tau) = 0.283(18)(37), \quad (4.7)$$

where the second error comes from the systematic error on the calibrating lattice spacing.

5. Discussion and conclusion

We should reemphasize that this is mainly a progress report. Most of the results reported here were performed on small volumes and with rather large quark masses. Our goal was to undertake a first exploration of the parameter space. It turned out that the results seem to make sense. The rather smooth junction of the α_s points from three different lattices show that overwhelming ultraviolet or infrared lattice artifacts are absent.

The points from different lattices with identical momenta do coincide unless $(L\mu)^2/(4\pi^2) \lesssim 2$. Suffering presumably from strong finite volume effects these points have been excluded from the global fits. The comparison at $\beta = 5.6, \kappa_{\text{sea}} = 0.1560$ of the 16^4 and the 24^4 volumes are encouraging and should be extended to other sets $(\beta, \kappa_{\text{sea}})$. The finite volume effect on masses seems to be well accounted for by eqs. (3.4), (3.5), and the good agreement of $m_{P,\infty}$ with the estimate in [9], performed on a larger time interval, confirms this optimism.

Our result for $\alpha_s(M_Z)$ is about 2 standard deviations below the world average experimental $\alpha_s(M_Z) = 0.119(2)$ [13]. It is slightly larger, although compatible within errors, with the result¹² of [10]: $\alpha_s(M_Z) = 0.1076(20)(18)$. Older results using NRQCD were closer to experiment: $\alpha_s^{(5)}(M_Z) = 0.1174(24)$ [8], $\alpha_s^{(5)}(M_Z) = 0.118(17)$ [9]. Our result for $\alpha_{s,\text{pert}}(M_\tau)$ is also 2 σ 's below the experimental value of $0.334(22)$ MeV [22]. However, the meaning of this comparison is unclear because we cannot take into account the non-perturbative contribution to $\alpha_s^{\overline{\text{MS}}}$ at M_τ .

We consider the fact that our preliminary result is 2 σ 's below experiment as very encouraging. We should stress that the error presented in eq. (4.7) corresponds to the statistical error and only to some systematic errors: mainly the choice of the fitting window and the calibration error. Other systematic effects should be systematically explored such as that of the dynamical-quark action and that of the mass of the dynamical-quark (ours are rather heavy). A calculation with a lighter dynamical-quark mass is in progress. As a final remark we would like to stress that our value for $\alpha_s(M_Z)$ is strongly correlated to the rather large $1/\mu^2$ corrections that we find in our fit. Starting from eq. (4.4) i.e. from a fit without power corrections we obtain $\alpha_s(M_Z) = 0.1211(3)(40)$. As already stated, in the fits, $\Lambda_{\overline{\text{MS}}}$ and c show an understandable tendency to vary a contrario. We are clearly encouraged to follow on this analysis and try to refine our result for $\alpha_s(M_Z)$.

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¹²This results from the fact that our value $\Lambda_{\overline{\text{MS}}}^{N_f=2} = 264(27)$ is larger than the value $217(16)(11)$ from [10].

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